Niall J English

List of Publications by Year
in descending order

263 papers	7,492 citations	43973 48 h-index	82410 72 g-index
266 all docs	266 docs citations	266 times ranked	6285 citing authors

#	Article	IF	Citations
1	Machine-learning-based many-body energy analysis of argon clusters: Fit for size?. Chemical Physics, 2022, 552, 111347.	0.9	3
2	Application of Porous Ceramics. Engineering Materials, 2022, , 499-537.	0.3	1
3	Characterization of Nanoporous Materials. Engineering Materials, 2022, , 319-351.	0.3	3
4	Electro-Oxidation Reaction of Methanol over La_{2â€“x}Sr_xNiO_{4+Î´} Ruddlesdenâ€“Popper Oxides. ACS Applied Energy Materials, 2022, 5, 503-515.	2.5	15
5	Effects of Externally Applied Electric Fields on the Manipulation of Solvated-Chignolin Folding: Static- versus Alternating-Field Dichotomy at Play. Journal of Physical Chemistry B, 2022, 126, 376-386.	1.2	4
6	A DFTB-Based Molecular Dynamics Investigation of an Explicitly Solvated Anatase Nanoparticle. Applied Sciences (Switzerland), 2022, 12, 780.	1.3	3
7	Improving Structural Stability and Anticoagulant Activity of a Thrombin Binding Aptamer by Aromatic Modifications. ChemBioChem, 2022, 23, .	1.3	1
8	Anti-gas hydrate surfaces: perspectives, progress and prospects. Journal of Materials Chemistry A, 2022, 10, 379-406.	5.2	14
9	Controlling hydrogen release from remaining-intact Clathrate hydrates by electromagnetic fields: molecular engineering via microsecond non-equilibrium molecular dynamics. RSC Advances, 2022, 12, 4370-4376.	1.7	4
10	Investigation of Dipolar Response of the Hydrated Hen-Egg White Lysozyme Complex under Externally Applied Electric Fields: Insights from Non-equilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2022, 126, 858-868.	1.2	4
11	Electric Field Effects on Photoelectrochemical Water Splitting: Perspectives and Outlook. Energies, 2022, 15, 1553.	1.6	2
12	Double Life of Methanol: Experimental Studies and Nonequilibrium Molecular-Dynamics Simulation of Methanol Effects on Methane-Hydrate Nucleation. Journal of Physical Chemistry C, 2022, 126, 6075-6081.	1.5	9
13	Sustainable Exploitation and Commercialization of Ultradense Nanobubbles: Reinventing Liquidity. ACS Sustainable Chemistry and Engineering, 2022, 10, 3383-3386.	3.2	7
14	Environmental Exploration of Ultra-Dense Nanobubbles: Rethinking Sustainability. Environments - MDPI, 2022, 9, 33.	1.5	8
15	Self-Diffusion of Individual Adsorbed Water Molecules at Rutile (110) and Anatase (101) TiO2 Interfaces from Molecular Dynamics. Crystals, 2022, 12, 398.	1.0	2
16	Understanding Competitive Photo-Induced Molecular Oxygen Dissociation and Desorption Dynamics atop a Reduced Rutile TiO₂(110) Surface: A Time-Domain Ab Initio Study. ACS Catalysis, 2022, 12, 6702-6711.	5.5	13
17	Thermodynamic evaluation of inhibitors for methane-hydrate formation. Fuel, 2022, 324, 124672.	3.4	7
18	Systematic Design-of-Experiments, factorial-design approaches for tuning simple empirical water models. Molecular Simulation, 2021, 47, 119-130.	0.9	1

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19	Diverse morphologies of zinc oxide nanoparticles and their electrocatalytic performance in hydrogen production. Journal of Energy Chemistry, 2021, 56, 162-170.	7.1	18
20	Influence of external static and alternating electric fields on self-diffusion of water from molecular dynamics. Journal of Molecular Liquids, 2021, 327, 114788.	2.3	12
21	A Review of Reactor Designs for Hydrogen Storage in Clathrate Hydrates. Applied Sciences (Switzerland), 2021, 11, 469.	1.3	13
22	Molecular Simulation of Crystallisation in External Electric Fields: A Review. Crystals, 2021, 11, 316.	1.0	3
23	Hydrogen and Deuterium Molecular Escape from Clathrate Hydrates: â€œLeakyâ€• Microsecond-Molecular-Dynamics Predictions. Journal of Physical Chemistry C, 2021, 125, 8430-8439.	1.5	4
24	A comprehensive review on the application of aerogels in CO2-adsorption: Materials and characterisation. Chemical Engineering Journal, 2021, 412, 128604.	6.6	92
25	Power-to-X: Lighting the Path to a Net-Zero-Emission Future. ACS Sustainable Chemistry and Engineering, 2021, 9, 7179-7181.	3.2	39
26	Structural and Electronic Properties of MgO/TiO₂ Interfaces: A First-Principles Molecular-Simulation Study. Journal of Physical Chemistry C, 2021, 125, 10795-10802.	1.5	2
27	Water Breakup at Fe₂O₃â€“Hematite/Water Interfaces: Influence of External Electric Fields from Nonequilibrium Ab Initio Molecular Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 6818-6826.	2.1	9
28	Donor-acceptor structure and dynamics: Molecular dynamics simulation study of TIP4P/2005 water model. Chemical Physics Letters, 2021, 775, 138581.	1.2	0
29	Electric-field-promoted photo-electrochemical production of hydrogen from water splitting. Journal of Molecular Liquids, 2021, 342, 116949.	2.3	11
30	The Importance of Precursors and Modification Groups of Aerogels in CO2 Capture. Molecules, 2021, 26, 5023.	1.7	12
31	In Situ Synchrotron X-ray Diffraction Studies of Hydrogen-Desorption Properties of 2LiBH4â€“Mg2FeH6 Composite. Molecules, 2021, 26, 4853.	1.7	0
32	Magnetic ferrite/carbonized cotton fiber composites for improving electromagnetic absorption properties at gigahertz frequencies. Journal of Materials Science and Technology, 2021, 86, 127-138.	5.6	29
33	Oxygen-evolution reactions (OER) on transition-metal-doped Fe₃Co(PO₄)₄ iron-phosphate surfaces: a first-principles study. Catalysis Science and Technology, 2021, 11, 4619-4626.	2.1	4
34	Hydrogen Inter-Cage Hopping and Cage Occupancies inside Hydrogen Hydrate: Molecular-Dynamics Analysis. Applied Sciences (Switzerland), 2021, 11, 282.	1.3	10
35	A C₃-symmetric twisted organic salt as an efficient mechano-/thermo-responsive molecule: a reusable and sensitive fluorescent thermometer. Chemical Communications, 2021, 57, 12321-12324.	2.2	6
36	Dielectric properties of ice VII under the influence of time-alternating external electric fields. Physical Chemistry Chemical Physics, 2021, , .	1.3	1

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37	Density of Phonon States in Cubic Ice Ic. Journal of Physical Chemistry C, 2021, 125, 23533-23538.	1.5	4
38	Microbial stabilisation and kinetic enhancement of marine methane hydrates in both deionised- and sea-water. Petroleum, 2021, , .	1.3	1
39	Crystallisation competition between cubic and hexagonal ice structures: molecular-dynamics insight. Molecular Simulation, 2021, 47, 18-26.	0.9	3
40	Intra-Cage Structure, Vibrations and Tetrahedral-Site Hopping of H2 and D2 in Doubly-Occupied 51264 Cages in sII Clathrate Hydrates from Path-Integral and Classical Molecular Dynamics. Applied Sciences (Switzerland), 2021, 11, 54.	1.3	3
41	Onset of anharmonicity and thermal conductivity in SnSe. Physical Review B, 2021, 104, .	1.1	5
42	Molecular Simulation of External Electric Fields on the Crystal State: A Perspective. Crystals, 2021, 11, 1405.	1.0	0
43	Unraveling Adhesion Strength between Gas Hydrate and Solid Surfaces. Langmuir, 2021, 37, 13873-13881.	1.6	14
44	Novel Superstructure-Phase Two-Dimensional Material 1T-VSe2 at High Pressure. Journal of Physical Chemistry Letters, 2020, 11, 380-386.	2.1	17
45	Microbial Stabilization and Kinetic Enhancement of Marine Methane Hydrates. Geomicrobiology Journal, 2020, 37, 279-286.	1.0	5
46	Infrared spectra and density of states at the interface between water and protein: Insights from classical molecular dynamics. Chemical Physics Letters, 2020, 757, 137867.	1.2	3
47	Kinetic study on electro-nucleation of water in a heterogeneous propane nano-bubble system to form polycrystalline ice Ic. Journal of Chemical Physics, 2020, 153, 084501.	1.2	4
48	Magnetic-Field Manipulation of Naturally Occurring Microbial Chiral Peptides to Regulate Gas-Hydrate Formation. Journal of Physical Chemistry Letters, 2020, 11, 9079-9085.	2.1	6
49	Self-ordering water molecules at TiO2 interfaces: Advances in structural classification. Journal of Chemical Physics, 2020, 153, 064502.	1.2	7
50	Hydrogen Storage in Propane-Hydrate: Theoretical and Experimental Study. Applied Sciences (Switzerland), 2020, 10, 8962.	1.3	6
51	Hydrogen Intramolecular Stretch Redshift in the Electrostatic Environment of Type II Clathrate Hydrates from SchrÃ¶dinger Equation Treatment. Applied Sciences (Switzerland), 2020, 10, 8504.	1.3	1
52	Thermal Conductivity of High-Temperature Phases of Cu2S from Ab Initio Molecular Dynamics: Advent of Lattice-Site Hopping. Journal of Physical Chemistry C, 2020, 124, 12318-12323.	1.5	0
53	Temperature-dependent kinetic pathways featuring distinctive thermal-activation mechanisms in structural evolution of ice VII. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 15437-15442.	3.3	9
54	Gas hydrates in sustainable chemistry. Chemical Society Reviews, 2020, 49, 5225-5309.	18.7	443

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55	Engineering Peptides to Catalyze and Control Stabilization of Gas Hydrates: Learning From Nature. Journal of Physical Chemistry Letters, 2020, 11, 5068-5075.	2.1	11
56	Dynamical properties of organo lead-halide perovskites and their interfaces to titania: insights from Density Functional Theory. Heliyon, 2020, 6, e03427.	1.4	4
57	Dynamical and structural properties of adsorbed water molecules at the TiO2 rutile-(110) surface: interfacial hydrogen bonding probed by ab-initio molecular dynamics. Molecular Physics, 2020, 118, e1725166.	0.8	4
58	In Situ Formation of Metal Hydrides Inside Carbon Aerogel Frameworks for Hydrogen Storage Applications. Journal of Carbon Research, 2020, 6, 38.	1.4	3
59	Dynamical and structural properties of adsorbed water molecules at the TiO2 anatase-(1Â0Â1) surface: Importance of interfacial hydrogen-bond rearrangements. Chemical Physics Letters, 2020, 743, 137164.	1.2	6
60	Stability-Ranking of Crystalline Ice Polymorphs Using Density-Functional Theory. Crystals, 2020, 10, 40.	1.0	2
61	Relaxation dynamics and power spectra of liquid water: a molecular dynamics simulation study. Molecular Physics, 2020, 118, e1733117.	0.8	0
62	First-principles studies on Î±-Fe₂O₃ surface slabs and mechanistic elucidation of a g-C₃N₄/Î±-Fe₂O₃ heterojunction. Catalysis Science and Technology, 2020, 10, 1376-1384.	2.1	20
63	First-principles study of the structural, electronic, magnetic properties of orthorhombic PrCuO3 perovskites. Chemical Physics Letters, 2020, 743, 137166.	1.2	2
64	Massive generation of metastable bulk nanobubbles in water by external electric fields. Science Advances, 2020, 6, eaaz0094.	4.7	72
65	Triplet Harvesting Using Two-Photon Absorption in Substituted Naphthalimides for Their Application as Heavy-Atom-Free Photosensitizers. Journal of Physical Chemistry C, 2020, 124, 8178-8185.	1.5	22
66	Possibility of realizing superionic ice VII in external electric fields of planetary bodies. Science Advances, 2020, 6, eaaz2915.	4.7	18
67	A New Relatively Simple Approach to Multipole Interactions in Either Spherical Harmonics or Cartesians, Suitable for Implementation into Ewald Sums. International Journal of Molecular Sciences, 2020, 21, 277.	1.8	6
68	Vibrational Spectra of a N719-Chromophore/Titania Interface from Empirical-Potential Molecular-Dynamics Simulation, Solvated by a Room Temperature Ionic Liquid. Journal of Visualized Experiments, 2020, , .	0.2	0
69	Classical and path-integral molecular-dynamics study on liquid water and ice melting using non-empirical TTM2.1-F model. Molecular Physics, 2019, 117, 3241-3253.	0.8	1
70	Opto-electronic properties of stable blue photosensitisers on a TiO2 anatase-101 surface for efficient dye-sensitised solar cells. Chemical Physics Letters, 2019, 731, 136624.	1.2	15
71	Hybrid versus global thermostatting in molecular-dynamics simulation of methane-hydrate crystallisation. Chinese Journal of Chemical Engineering, 2019, 27, 2180-2188.	1.7	3
72	Acoustic-propagation properties of methane clathrate hydrates from non-equilibrium molecular dynamics. Journal of Chemical Physics, 2019, 151, 144505.	1.2	8

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73	Electric-Field Control of Neon Uptake and Release to and from Clathrate Hydrates. Journal of Physical Chemistry C, 2019, 123, 27554-27560.	1.5	10
74	Atmospheric oxidation mechanism and kinetics of 2-bromo-4,6-dinitroaniline by OH radicals â€“ a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 21109-21127.	1.3	0
75	Magnetic-field effects on methane-hydrate kinetics and potential geophysical implications: Insights from non-equilibrium molecular dynamics. Science of the Total Environment, 2019, 661, 664-669.	3.9	8
76	Controlling ionic conductivity through transprotein electropores in human aquaporin 4: a non-equilibrium molecular-dynamics study. Physical Chemistry Chemical Physics, 2019, 21, 3339-3346.	1.3	15
77	Hydrogen-/propane-hydrate decomposition: thermodynamic and kinetic analysis. Molecular Physics, 2019, 117, 2434-2442.	0.8	9
78	Crystal Structure Prediction via Basin-Hopping Global Optimization Employing Tiny Periodic Simulation Cells, with Application to Waterâ€“Ice. Journal of Chemical Theory and Computation, 2019, 15, 3889-3900.	2.3	13
79	Orientational and Folding Thermodynamics via Electric Dipole Moment Restraining. Journal of Physical Chemistry B, 2019, 123, 2599-2608.	1.2	5
80	Mechanisms of Iodideâ€“Triiodide Exchange Reactions in Ionic Liquids: A Reactive Molecular-Dynamics Exploration. International Journal of Molecular Sciences, 2019, 20, 1123.	1.8	5
81	Amplitude effects on seismic velocities: How low can we go?. Journal of Chemical Physics, 2019, 150, 084101.	1.2	1
82	Ionic conductivity along transmembrane-electropores in human aquaporin 4: calcium effects from non-equilibrium molecular dynamics. Molecular Physics, 2019, 117, 3783-3790.	0.8	3
83	Electro-nucleation of water nano-droplets in No Man's Land to fault-free ice I_c. Physical Chemistry Chemical Physics, 2018, 20, 8042-8053.	1.3	17
84	Electro-suppression of water nano-dropletsâ€™ solidification in no manâ€™s land: Electromagnetic fieldsâ€™ entropic trapping of supercooled water. Journal of Chemical Physics, 2018, 148, 044503.	1.2	6
85	Elastic Characterization of S- and P-Wave Velocities in Marinelike Silica: The Role of Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2018, 122, 3006-3013.	1.5	2
86	Study of hydrogen-molecule guests in type II clathrate hydrates using a force-matched potential model parameterised from ab initio molecular dynamics. Journal of Chemical Physics, 2018, 148, 102323.	1.2	18
87	Silicon-bridged triphenylamine-based organic dyes for efficient dye-sensitised solar cells. Solar Energy, 2018, 160, 64-75.	2.9	18
88	Thermal Conductivity of Solids from First-Principles Molecular Dynamics Calculations. Journal of Physical Chemistry C, 2018, 122, 10682-10690.	1.5	16
89	Molecular Dynamics Study of Propane Hydrate Dissociation: Nonequilibrium Analysis in Externally Applied Electric Fields. Journal of Physical Chemistry C, 2018, 122, 7504-7515.	1.5	31
90	Molecular-dynamics study of propane-hydrate dissociation: Fluctuation-dissipation and non-equilibrium analysis. Journal of Chemical Physics, 2018, 148, 114504.	1.2	25

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91	A systematic study via ab-initio MD of the effect solvation by room temperature ionic liquid has on the structure of a chromophore-titania interface. Computational Materials Science, 2018, 141, 193-206.	1.4	4
92	System-density fluctuations and electro-dissociation of methane clathrate hydrates in externally-applied static electric fields. Journal of Chemical Thermodynamics, 2018, 117, 68-80.	1.0	30
93	Vibrational Study of Iodide-Based Room-Temperature Ionic-Liquid Effects on Candidate N719-Chromophore/Titania Interfaces for Dye-Sensitised Solar-Cell Applications from Ab-Initio Based Molecular-Dynamics Simulation. Energies, 2018, 11, 2570.	1.6	2
94	Ab Initio Molecular Dynamics Studies of the Effect of Solvation by Room-Temperature Ionic Liquids on the Vibrational Properties of a N719-Chromophore/Titania Interface. Journal of Physical Chemistry C, 2018, 122, 26464-26471.	1.5	3
95	Transprotein-Electropore Characterization: A Molecular Dynamics Investigation on Human AQP4. ACS Omega, 2018, 3, 15361-15369.	1.6	20
96	Human aquaporin 4 gating dynamics under axially oriented electric-field impulses: A non-equilibrium molecular-dynamics study. Journal of Chemical Physics, 2018, 149, 245102.	1.2	23
97	Does Local Structure Bias How a Crystal Nucleus Evolves?. Journal of Physical Chemistry Letters, 2018, 9, 6991-6998.	2.1	19
98	Vibrational, energetic-dynamical and dissociation properties of water clusters in static electric fields: Non-equilibrium molecular-dynamics insights. Chemical Physics Letters, 2018, 710, 207-214.	1.2	7
99	Non-equilibrium molecular-dynamics study of electromagnetic-field-induced propane-hydrate dissociation. Journal of Chemical Physics, 2018, 149, 124702.	1.2	20
100	Pressure-Induced Densification of Ice I_h under Triaxial Mechanical Compression: Dissociation versus Retention of Crystallinity for Intermediate States in Atomistic and Coarse-Grained Water Models. Journal of Physical Chemistry Letters, 2018, 9, 5267-5274.	2.1	7
101	Elucidating mysteries of phase-segregated membranes: mobile-lipid recruitment facilitates poresâ€™ passage to the fluid phase. Physical Chemistry Chemical Physics, 2018, 20, 19234-19239.	1.3	4
102	Pressure dependence of structural properties of ice VII: An ab initio molecular-dynamics study. Journal of Chemical Physics, 2018, 148, 204505.	1.2	7
103	Tweaking the Electronic and Optical Properties of Î±-MoO3 by Sulphur and Selenium Doping â€“ a Density Functional Theory Study. Scientific Reports, 2018, 8, 10144.	1.6	25
104	Formation and properties of water from quartz and hydrogen at high pressure and temperature. Earth and Planetary Science Letters, 2017, 461, 54-60.	1.8	13
105	Vibrational Modes of Hydrogen Hydrates: A First-Principles Molecular Dynamics and Raman Spectra Study. Journal of Physical Chemistry C, 2017, 121, 3690-3696.	1.5	29
106	Hydrogen-bond dynamics at the bioâ€“water interface in hydrated proteins: a molecular-dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 318-329.	1.3	28
107	On the Mechanism of the Iodideâ€“Triiodide Exchange Reaction in a Solid-State Ionic Liquid. Journal of Physical Chemistry B, 2017, 121, 6436-6441.	1.2	8
108	Ice-Amorphization of Supercooled Water Nanodroplets in No Manâ€™s Land. ACS Earth and Space Chemistry, 2017, 1, 187-196.	1.2	11

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109	Exploring Rutile (110) and Anatase (101) TiO₂ Water Interfaces by Reactive Force-Field Simulations. Journal of Physical Chemistry C, 2017, 121, 6701-6711.	1.5	41
110	Quantum and classical inter-cage hopping of hydrogen molecules in clathrate hydrate: temperature and cage-occupation effects. Physical Chemistry Chemical Physics, 2017, 19, 717-728.	1.3	28
111	Mechanisms and Nucleation Rate of Methane Hydrate by Dynamical Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry C, 2017, 121, 24223-24234.	1.5	30
112	Electropumping of Water Through Human Aquaporin 4 by Circularly Polarized Electric Fields: Dramatic Enhancement and Control Revealed by Non-Equilibrium Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 4646-4651.	2.1	11
113	Global-density fluctuations in methane clathrate hydrates in externally applied electromagnetic fields. Journal of Chemical Physics, 2017, 147, 024506.	1.2	22
114	Communication: Influence of external static and alternating electric fields on water from long-time non-equilibrium ab initio molecular dynamics. Journal of Chemical Physics, 2017, 147, 031102.	1.2	57
115	optPBE-vdW density functional theory study of liquid water and pressure-induced structural evolution in ice Ih. Canadian Journal of Chemistry, 2017, 95, 1205-1211.	0.6	6
116	Equilibrium Born-Oppenheimer molecular-dynamics exploration of the lattice thermal conductivity of silicon clathrates. Computational Materials Science, 2017, 126, 1-6.	1.4	9
117	Understanding the interface between silicon-based materials and water: Molecular-dynamics exploration of infrared spectra. AIP Advances, 2017, 7, .	0.6	20
118	Exploring Promising Catalysts for Chemical Hydrogen Storage in Ammonia Borane: A Density Functional Theory Study. Catalysts, 2017, 7, 140.	1.6	11
119	Organic Dyes Containing Coplanar Dihexyl-Substituted Dithienosilole Groups for Efficient Dye-Sensitised Solar Cells. International Journal of Photoenergy, 2017, 2017, 1-14.	1.4	8
120	Dynamics of hydrogen guests in ice XVII nanopores. Physical Review Materials, 2017, 1, .	0.9	9
121	Human Aquaporin 4 Gating Dynamics under Perpendicularly-Oriented Electric-Field Impulses: A Molecular Dynamics Study. International Journal of Molecular Sciences, 2016, 17, 1133.	1.8	22
122	Diffusivity and Mobility of Adsorbed Water Layers at TiO2 Rutile and Anatase Interfaces. Crystals, 2016, 6, 1.	1.0	72
123	Near-microsecond human aquaporin 4 gating dynamics in static and alternating external electric fields: Non-equilibrium molecular dynamics. Journal of Chemical Physics, 2016, 145, 085102.	1.2	13
124	Perturbation of hydration layer in solvated proteins by external electric and electromagnetic fields: Insights from non-equilibrium molecular dynamics. Journal of Chemical Physics, 2016, 145, 205101.	1.2	10
125	Study of clathrate hydrates via equilibrium molecular-dynamics simulation employing polarisable and non-polarisable, rigid and flexible water models. Journal of Chemical Physics, 2016, 144, 164503.	1.2	25
126	Electromagnetic-field effects on structure and dynamics of amyloidogenic peptides. Journal of Chemical Physics, 2016, 144, 085101.	1.2	46

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127	Oscillating electric-field effects on adsorbed-water at rutile- and anatase-TiO2 surfaces. Journal of Chemical Physics, 2016, 145, 204706.	1.2	18
128	Electric-Field Effects on Adsorbed-Water Structural and Dynamical Properties at Rutile- and Anatase-TiO₂ Surfaces. Journal of Physical Chemistry C, 2016, 120, 19603-19612.	1.5	42
129	Free-Energy Calculations of the Intercage Hopping Barriers of Hydrogen Molecules in Clathrate Hydrates. Journal of Physical Chemistry C, 2016, 120, 16561-16567.	1.5	40
130	Role of Hydration Layer in Dynamical Transition in Proteins: Insights from Translational Self-Diffusivity. Journal of Physical Chemistry B, 2016, 120, 12031-12039.	1.2	14
131	Time-dependent density fluctuations in liquid water. Chemical Physics Letters, 2016, 649, 119-122.	1.2	2
132	Structural and dynamical properties of methane clathrate hydrates from molecular dynamics: Comparison of atomistic and more coarse-grained potential models. Fluid Phase Equilibria, 2016, 413, 235-241.	1.4	8
133	Dispersion and Solvation Effects on the Structure and Dynamics of N719 Adsorbed to Anatase Titania (101) Surfaces in Room-Temperature Ionic Liquids: An ab Initio Molecular Simulation Study. Journal of Physical Chemistry C, 2016, 120, 21-30.	1.5	9
134	Verhulst and stochastic models for comparing mechanisms of MAb productivity in six CHO cell lines. Cytotechnology, 2016, 68, 1499-1511.	0.7	2
135	Distortion induced magnetic phase transition in cubic BaFeO 3. Journal of Magnetism and Magnetic Materials, 2016, 401, 1097-1105.	1.0	7
136	Communication: Librational dynamics in water, sI and sII clathrate hydrates, and ice Ih: Molecular-dynamics insights. Journal of Chemical Physics, 2016, 144, 051101.	1.2	13
137	Massively parallel molecular dynamics simulation of formation of ice-crystallite precursors in supercooled water: Incipient-nucleation behavior and role of system size. Physical Review E, 2015, 92, 032132.	0.8	13
138	Hydrogen-bond vibrational and energetic dynamical properties in sI and sII clathrate hydrates and in ice Ih: Molecular dynamics insights. Journal of Chemical Physics, 2015, 143, 154504.	1.2	7
139	Structural Properties of Liquid Water and Ice Ih from Ab-Initio Molecular Dynamics with a Non-Local Correlation Functional. Energies, 2015, 8, 9383-9391.	1.6	20
140	Electric field-controlled semiconductor nanorod assembly in solution: mechanistic insights from non-equilibrium molecular dynamics. Canadian Journal of Chemistry, 2015, 93, 888-890.	0.6	2
141	Ternary structure reveals mechanism of a membrane diacylglycerol kinase. Nature Communications, 2015, 6, 10140.	5.8	30
142	Photophysics, photochemistry and thermal stability of diarylethene-containing benzothiazolium species. Journal of Photochemistry and Photobiology A: Chemistry, 2015, 301, 20-31.	2.0	5
143	Modelling of Mammalian Cell Cultures. Cell Engineering, 2015, , 259-326.	0.4	9
144	Prediction of Henryâ€™s Law Constants via group-specific quantitative structure property relationships. Chemosphere, 2015, 127, 1-9.	4.2	12

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145	Communication: Influence of nanosecond-pulsed electric fields on water and its subsequent relaxation: Dipolar effects and debunking memory. Journal of Chemical Physics, 2015, 142, 141101.	1.2	23
146	Perspectives on external electric fields in molecular simulation: progress, prospects and challenges. Physical Chemistry Chemical Physics, 2015, 17, 12407-12440.	1.3	202
147	Clathrate structure-type recognition: Application to hydrate nucleation and crystallisation. Journal of Chemical Physics, 2015, 142, 244503.	1.2	33
148	Perspectives on molecular simulation of clathrate hydrates: Progress, prospects and challenges. Chemical Engineering Science, 2015, 121, 133-156.	1.9	168
149	Revisiting Verhulst and Monod models: analysis of batch and fed-batch cultures. Cytotechnology, 2015, 67, 515-530.	0.7	18
150	Massively parallel molecular-dynamics simulation of ice crystallisation and melting: The roles of system size, ensemble, and electrostatics. Journal of Chemical Physics, 2014, 141, 234501.	1.2	22
151	Dipolar response and hydrogen-bond kinetics in liquid water in square-wave time-varying electric fields. Molecular Physics, 2014, 112, 1870-1878.	0.8	44
152	Massively parallel molecular dynamics simulation of formation of clathrate-hydrate precursors at planar water-methane interfaces: Insights into heterogeneous nucleation. Journal of Chemical Physics, 2014, 140, 204714.	1.2	56
153	The influence of Ti- and Si-doping on the structure, morphology and photo-response properties of Î±-Fe2O3 for efficient water-splitting: Insights from experiment and first-principles calculations. Chemical Physics Letters, 2014, 592, 242-246.	1.2	18
154	Implicit and explicit solvent models for modeling a bifunctional arene ruthenium hydrogenâ€storage catalyst: A classical and ab initio molecular simulation study. Journal of Computational Chemistry, 2014, 35, 683-691.	1.5	6
155	Perspectives on atmospheric CO2 fixation in inorganic and biomimetic structures. Coordination Chemistry Reviews, 2014, 269, 85-95.	9.5	57
156	Towards the design of novel boronâ€and nitrogenâ€substituted ammoniaâ€borane and bifunctional arene ruthenium catalysts for hydrogen storage. Journal of Computational Chemistry, 2014, 35, 891-903.	1.5	7
157	Theoretical studies of separation of cisâ€“trans isomers using dinuclear (Cu2+- and Zn2+-based) cryptates. Journal of Molecular Modeling, 2014, 20, 2328.	0.8	1
158	Thermal Conductivity of Supercooled Water: An Equilibrium Molecular Dynamics Exploration. Journal of Physical Chemistry Letters, 2014, 5, 3819-3824.	2.1	15
159	Photo-active and dynamical properties of hematite (Fe2O3)â€“water interfaces: an experimental and theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 14445.	1.3	26
160	Methane Clathrate Hydrate Nucleation Mechanism by Advanced Molecular Simulations. Journal of Physical Chemistry C, 2014, 118, 22847-22857.	1.5	87
161	Reversible pressure-induced crystal-amorphous structural transformation in ice Ih. Chemical Physics Letters, 2014, 609, 54-58.	1.2	9
162	Density functional theory calculations of catalytic mechanistic pathways for the formation of O₂involving triazolylidene iridium complexes. New Journal of Chemistry, 2014, 38, 4060.	1.4	5

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163	Minimizing Electronâ€“Hole Recombination on TiO₂ Sensitized with PbSe Quantum Dots: Time-Domain Ab Initio Analysis. Journal of Physical Chemistry Letters, 2014, 5, 2941-2946.	2.1	63
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